

2-Nitropropane  
79-46-9 | DTXSID6020981

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.85            | 0.69 | 0.86           | 0.67 | 0.86       | 0.78 |

## Model Results

**Predicted value:** 1.03

**Global applicability domain:** Inside

**Local applicability domain index:** 6.93e-01

**Confidence level:** 8.92e-01

## Nearest Neighbors from the Training Set

Image not found

2-Nitropropane

**Measured:** 0.93

**Predicted:** 1.03

Image not found

1-Nitropropane

**Measured:** 0.87

**Predicted:** 9.14e-01

Image not found

1-Nitrobutane

**Measured:** 1.47

**Predicted:** 1.35

Image not found

Propane, 2-methyl-1-nitro-

**Measured:** 1.40

**Predicted:** 1.42

Image not found

2-Nitrobutane

**Measured:** 1.20

**Predicted:** 1.33